A NEW APPROACH TO THE LARGE-EDDY SIMULATION OF HIGH-SPEED COMPRESSIBLE FLOWS

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ABSTRACT

An entirely new approach to the large-eddy simulation (LES) of high-speed compressible turbulent flows is presented. In this new approach to large-eddy simulations, subgrid scale stress models go continuously to Reynolds stress models in the coarse mesh/infinite Reynolds number limit, where a Reynolds stress calculation (RANS) is done in parallel with the LES to get an estimate of the Kolmogorov length scale. Hence, this formally constitutes a combined LES/time-dependent RANS capability. Here, the Reynolds stress model that is recovered in the coarse mesh limit has a dependence on rotational strains through strain-dependent coefficients as well as through anisotropic eddy viscosity terms which are usually neglected in subgrid scale models. Unlike in existing subgrid scale models, this new model has the correct dependence on the mesh size through the dimensionless ratio of the computational mesh size to the Kolmogorov length scale. It is this ratio that determines how well-resolved a computation is in the numerical simulation of turbulence and should be used to parameterize subgid scale models. Use is made of the Morkovin hypothesis in the formulation of compressible subgrid scale models. This allows for the description of supersonic turbulent flows provided that they are not in the hypersonic flow regime. A critical assessment of this new approach is provided along with a discussion of traditional approaches and the prospects for future applications to the high-speed compressible flows of technological importance.

1. INTRODUCTION

Large-eddy simulations of turbulence have been a popular tool in turbulence research since the ground-breaking work of Smagorinsky (1963) three decades ago. In large-eddy simulations (LES), the large, energy containing eddies are computed directly while the small scales are modeled since they are believed to be more universal in character (see Rogallo and Moin 1984 for an interesting review). Large-eddy simulations were first used in meteorological computations over thirty years ago. However, this was largely within the context of incompressible flow. On the other hand, the first complete large-eddy simulation of a high-speed compressible turbulent flow was probably conducted by Erlebacher, *et al* (1992) less than a decade ago. This, however, was based on a variable density extension of the Smagorinsky model which was used with the scale-similarity model to form a compressible version of the linear combination model (see Bardina, Ferziger and Reynolds 1983). Thus, these simulations were, to a large extent, based on the Smagorinsky model which has a variety of problems associated with it (see Speziale 1997a). For example, the Smagorinsky model depends on the dimensional mesh size Δ so that the subgrid scale stress tensor $\tau_{ij} \to \infty$ as $\Delta \to \infty$. Hence, a badly calibrated Reynolds stress model – that is overly dissipative – is recovered in the coarse mesh limit. Furthermore, the Smagorinsky model has no dependence on rotational strains and contains no anisotropic eddy viscosity terms. This makes it impossible to properly describe rotating turbulent flows; rotations substantially impede the cascade which requires subgrid scale models to become substantially less dissipative in the rapid rotation limit. In addition, the anisotropic eddy viscosity terms are needed to account for backscatter effects since they are dispersive in character. Thus, a new approach to LES is needed that transcends the Smagorinsky model and is, furthermore, more suitable for compressible LES. This forms the motivation for the present paper.

An entirely new approach to compressible large-eddy simulations will be presented in this paper. This approach will require that a Reynolds stress calculation (RANS) be conducted in parallel with the LES in order to get an estimate of the Kolmogorov length scale (a subgrid scale stress model will be developed that depends on the ratio of the computational mesh size to the Kolmogorov length scale which is the parameter that determines how well resolved a turbulent flow is). This only adds, at most, on the average 10% to the computational expense. Since, the Reynolds-averaged turbulent kinetic energy and dissipation rate need to be obtained anyhow, they are used to partially parameterize the constants of the model and to non-dimensionalize the strain rates. Furthermore, it should be noted that since the turbulent dissipation rate is raised to the 1/4 power in the definition of the Kolmogorov length scale, it is quite feasible to get a good estimate of this quantity with the current generation of Reynolds stress models where it only needs to be calculated to within 50%. The subgrid scale kinetic energy and dissipation rate can vary too much locally and, thus, are not that suitable for this purpose. In addition, this allows subgrid scale stress models to go more continuously to Reynolds stress models in the coarse mesh limit. The main purpose of this new approach is to develop subgrid scale stress models that go continuously to state-of-the-art Reynolds stress models in the coarse mesh limit. Here, the anisotropic eddy viscosity of an explicit algebraic stress model (see Gatski and Speziale 1993) will be used for this purpose (this formally constitutes a two-equation model). The anisotropic eddy viscosity terms are dispersive in character and can account for backscatter effects. Furthermore, unlike in the Smagorinsky model or most other subgrid scale stress models, the coefficients of the model depend on both the irrotational and rotational strain rate invariants which allows for a better description of rotating flows. Of course, in the fine mesh limit as the computational mesh size $\Delta \to 0$, the subgrid scale stress tensor $\tau_{ij} \to 0$ – as with existing subgrid scale stress models such as the Smagorinsky model – so that a direct numerical simulation (DNS) is recovered. However, this dependence is more properly parameterized by the ratio of the computational mesh size to the Kolmogorov length scale as discussed above.

As far as compressibility effects are concerned, the Morkovin hypothesis will be made use of (see Morkovin 1964). In the Morkovin hypothesis, it is assumed that compressibility effects only enter into the description of the turbulence quantities through changes in the mean density (also see Cebeci and Smith 1974). The Morkovin hypothesis has been validated in wall-bounded turbulent flows, provided they are not in the hypersonic flow regime where the external Mach number $Ma_\infty > 5$. For the flat plate turbulent boundary layer, it is approximately valid for external Mach numbers $Ma_\infty < 8$ (see Zhang, So, Speziale and Lai 1993). Since the external Mach number is somewhat less at the subgrid scale level, the Morkovin hypothesis is probably a good approximation for the development of subgrid scale models, in general turbulent flows, for external Mach numbers $Ma_\infty < 8$. Thus, the supersonic flow regime – as well as the beginning part of the hypersonic flow regime – can be well described by this hypothesis. Of course, this hypothesis breaks down entirely in strongly hypersonic flows where real gas effects and dissociation must be accounted for. Turbulent dilatational effects – which are neglected in the Morkovin hypothesis – must also be accounted for in compressible turbulent flows where the external Mach number Ma_∞ is greater than 4 or 5 (more precisely, when the turbulence Mach number, which will be discussed later, is greater than approximately 0.3). While the inclusion of the dilatational dissipation can be useful in free turbulent shear flows for large Mach numbers (see Sarkar, Erlebacher, Hussaini and Kreiss 1991 and Zeman 1990), it is counterproductive in wall-bounded turbulent flows where it can cause a degradation of the predictions. Thus, turbulent dilatational models will not be made full use of here for the development of subgrid scale models.

The subgrid scale modeling for this combined LES/time-dependent RANS capability will be discussed in detail in the sections to follow. It has the potential to bridge the gap between DNS, LES and RANS. A full discussion of the implications for turbulence research will be provided in the last section.

2. A REVIEW OF COMPRESSIBLE LARGE-EDDY SIMULATIONS

The full equations of motion for an ideal gas will be considered (cf. Cebeci and Smith 1974):

Continuity

$$\frac{\partial \rho}{\partial t} + (\rho u_i)_{,i} = 0 \tag{1}$$

Momentum

$$\frac{\partial}{\partial t}(\rho u_i) + (\rho u_i u_j)_{,j} = -p_{,i} + \sigma_{ij,j} \tag{2}$$

$$[\sigma_{ij} = -\frac{2}{3}\mu u_{k,k}\delta_{ij} + \mu(u_{i,j} + u_{j,i})]$$

Energy

$$\frac{\partial}{\partial t}(\rho C_v T) + (\rho u_i C_v T)_{,i} = -p u_{i,i} + \Phi + (\kappa T_{,i})_{,i} \tag{3}$$

$$[\Phi \equiv \sigma_{ij} u_{i,j} = -\frac{2}{3}\mu(u_{i,i})^2 + \mu(u_{i,j} + u_{j,i})u_{i,j}]$$

State

$$p = \rho R T \tag{4}$$

where

ρ	$\equiv$	mass density
u_i	$\equiv$	velocity vector
p	$\equiv$	thermodynamic pressure
μ	$\equiv$	dynamic viscosity
σ_{ij}	$\equiv$	viscous stress tensor
T	$\equiv$	absolute temperature
κ	$\equiv$	thermal conductivity
R	$\equiv$	ideal gas constant
C_v	$\equiv$	specific heat at constant volume
Φ	$\equiv$	viscous dissipation function
$(\ )_{,i}$	$\equiv$	$\frac{\partial}{\partial x_i}(\ )$.

For any flow variable $\mathcal{F}$, we can introduce the decomposition

$$\mathcal{F} = \overline{\mathcal{F}} + \mathcal{F}' \tag{5}$$

where $\overline{\mathcal{F}}$ is a standard filter and a prime represents a subgrid scale fluctuation. These, respectively, represent the large and small scale fields of the turbulence. Alternatively, the decomposition

$$\mathcal{F} = \tilde{\mathcal{F}} + \mathcal{F}'' \tag{6}$$

can be introduced where

$$\tilde{\mathcal{F}} = \frac{\overline{\rho\mathcal{F}}}{\overline{\rho}} \tag{7}$$

is the Favre (or mass-weighted) filter. Here,

$$\overline{\mathcal{F}'} \neq 0, \ \widetilde{\mathcal{F}''} \neq 0$$

and

$$\tilde{\mathcal{F}}' \neq 0, \ \overline{\mathcal{F}}'' \neq 0,$$

in general. A filtered quantity is given by

$$\overline{\mathcal{F}} = \int_D G(\mathbf{x} - \mathbf{x}^*, \Delta)\mathcal{F}(\mathbf{x}^*)d^3x^* \tag{8}$$

In (8), Δ is the computational mesh size and G is a filter function which is normalized as follows:

$$\int_D G(\mathbf{x} - \mathbf{x}^*, \Delta)d^3x^* = 1. \tag{9}$$

This guarantees that G becomes a Dirac delta sequence in the limit as $\Delta \to 0$:

$$\lim_{\Delta \to 0} \int_D G(\mathbf{x} - \mathbf{x}^*, \Delta)\phi(\mathbf{x}^*)d^3x^* = \int_D \delta(\mathbf{x} - \mathbf{x}^*)\phi(\mathbf{x}^*)d^3x^* \equiv \phi(\mathbf{x})$$

where $\delta(\mathbf{x} - \mathbf{x}^*)$ is the Dirac delta function. Direct numerical simulations (DNS) are, thus, recovered in the fine mesh limit. Due to the Riemann-Lebesgue Theorem, (8) substantially reduces the amplitude of the high-wavenumber Fourier components in space of any flow variable $\mathcal{F}$ (consequently, $\overline{\mathcal{F}}$ represents the large scale part of $\mathcal{F}$). The filter function G has usually been taken to be a Gaussian filter in infinite domains or a piecewise continuous distribution of bounded support in compact domains (in the latter case, the simple box filter has been commonly used with finite difference methods; see Deardorff 1970). The box filter on a non-uniform mesh is given by

$$G(\mathbf{x} - \mathbf{x}^*, \Delta) = \begin{cases} 1/8\Delta^3, & |x_i - x_i{}^*| \leq \Delta_{x_i} \\ 0, & |x_i - x_i{}^*| > \Delta_{x_i} \end{cases} \tag{10}$$

for $i = 1, 2, 3$ where Δ_{x_i}, is Δ_x, Δ_y and Δ_z, respectively, and where Δ is given by

$$\Delta = (\Delta_x \Delta_y \Delta_z)^{1/3}$$

(Δ_x, Δ_y and Δ_z are the mesh sizes in the x, y and z directions, respectively, obtained after a coordinate transformation).

The filtered continuity, momentum and energy equations take the form

Continuity

$$\frac{\partial \overline{\rho}}{\partial t} + (\overline{\rho} \tilde{u}_i)_{,i} = 0 \tag{11}$$

Momentum

$$\frac{\partial}{\partial t}(\overline{\rho}\tilde{u}_i) + (\overline{\rho}\tilde{u}_i\tilde{u}_j)_{,j} = -\overline{p}_{,i} + \overline{\sigma}_{ij,j} - (\overline{\rho}\tau_{ij})_{,j} \tag{12}$$

$$(\tau_{ij} \equiv \widetilde{u_i'' u_j''},\ \overline{p} = \overline{\rho} R \tilde{T})$$

Energy

$$\begin{aligned} \frac{\partial}{\partial t}(\overline{\rho}\overline{C}_v\tilde{T}) + (\rho\tilde{u}_i\overline{C}_v\tilde{T})_{,i} &= -\overline{p}\tilde{u}_{i,i} - \overline{p}\overline{u''_{i,i}} \\ &-\overline{p' u'_{i,i}} + \overline{\Phi} + (\overline{\kappa T_{,i}})_{,i} - Q_{i,i} \\ &(Q_i \equiv \overline{\rho}\overline{C}_v \widetilde{u_i'' T''}) \end{aligned} \tag{13}$$

where turbulent fluctuations in C_v have been neglected. Here, τ_{ij} is the Favre-filtered subgrid scale stress tensor and Q_i is the Favre-filtered subgrid scale Reynolds heat flux; $\overline{\Phi}$ is the filtered dissipation function. The filtered dissipation function is given by:

$$\begin{aligned} \overline{\Phi} &= \overline{\sigma}_{ij}\overline{u}_{i,j} + \overline{\sigma'_{ij} u'_{i,j}} \\ &= \overline{\sigma}_{ij}\tilde{u}_{i,j} + \overline{\sigma}_{ij}\overline{u''_{i,j}} + \overline{\rho}\varepsilon \end{aligned} \tag{14}$$

where $\varepsilon \equiv \overline{\sigma'_{ij} u'_{i,j}}/\overline{\rho}$ is the filtered turbulent dissipation rate. Hence, $\overline{\Phi} \to \overline{\rho}\varepsilon$ as the Reynolds number $Re \to \infty$.

In high-Reynolds-number turbulent flows, the molecular diffusion terms are dominated by the turbulent transport terms except in a thin sublayer near walls. If we assume in this region that fluctuations in the viscosity, thermal conductivity and density can be neglected we can then make the approximations:

$$\begin{aligned} \overline{\sigma}_{ij} &\equiv -\frac{2}{3}\overline{\mu u_{k,k}}\delta_{ij} + \overline{\mu(u_{i,j} + u_{j,i})} \\ &\approx -\frac{2}{3}\overline{\mu}\tilde{u}_{k,k}\delta_{ij} + \overline{\mu}(\tilde{u}_{i,j} + \tilde{u}_{j,i}) \end{aligned}$$

$$\overline{q}_i \equiv -\overline{\kappa T_{,i}} \approx -\overline{\kappa}\tilde{T}_{,i}.$$

Thus, in order to achieve closure, models are needed for:

(1) The Favre-filtered subgrid scale Reynolds stress, τ_{ij}

(2) The Favre-filtered subgrid scale Reynolds heat flux, Q_i

(3) The subgrid scale mass flux, $\overline{u_i''}$

(4) The subgrid scale dissipation rate, ε

(5) The subgid scale pressure-dilatation correlation, $\overline{p' u'_{i,i}}$.

This makes the problem of conducting compressible large-eddy simulations far more difficult than its incompressible counterpart.

The full form of the subgrid scale stress tensor is given by

$$\tau_{ij} = L_{ij} + C_{ij} + R_{ij} \tag{15}$$

where

$$L_{ij} \equiv \widetilde{\tilde{u}_i \tilde{u}_j} - \tilde{u}_i \tilde{u}_j \tag{16}$$

$$C_{ij} \equiv \widetilde{\tilde{u}_i u_j''} + \widetilde{u_i'' \tilde{u}_j} \tag{17}$$

$$R_{ij} \equiv \widetilde{u_i'' u_j''} \tag{18}$$

are, respectively, the Leonard stresses, subgrid scale cross stresses and subgrid scale Reynolds stresses (see Leonard 1974 and Ferziger 1976).

The Smagorinsky model has been used for either the entire deviatoric subgrid scale stress tensor or for the deviatoric part of the subgrid scale Reynolds stress tensor. In the latter case, for compressible flows, the deviatoric part of the Reynolds subgrid scale stress tensor is modeled as

$$_D R_{ij} = -2C_s^2 \Delta^2 (2\tilde{S}_{kl}\tilde{S}_{kl})^{1/2} (\tilde{S}_{ij} - \frac{1}{3}\tilde{S}_{mm}\delta_{ij}) \tag{19}$$

where

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

is the rate of strain tensor. In the incompressible limit, $\tilde{S}_{ij} \to \overline{S}_{ij}$ and, furthermore,

$$\tilde{S}_{mm} = \nabla \cdot \overline{\mathbf{u}} = 0 \tag{20}$$

so that the incompressible form of the Smagorinsky model is recovered. Here, C_s is the Smagorinsky constant that assumes the approximate value of 0.1 in many flows but can vary by as much as a factor of three. When the Smagorinsky model is used for the subgrid scale Reynolds stress tensor it is usually used in conjunction with the scale similarity model for the subgrid scale Leonard and cross stresses given by (see Bardina, Ferziger and Reynolds 1983)

$$L_{ij} + C_{ij} = \widetilde{\tilde{u}_i \tilde{u}_j} - \tilde{\tilde{u}}_i \tilde{\tilde{u}}_j \tag{21}$$

whose coefficient is unity in order to preserve Galilean invariance (see Speziale 1985). Biringen and Reynolds (1981) and Moin and Kim (1982) had violated Galilean invariance by applying the Smagorinsky model to the sum of the cross stresses and Reynolds subgrid scale stresses (see Speziale 1985).

The subgrid scale Reynolds stress tensor can be split into isotropic and deviatoric parts as follows:

$$R_{ij} = \frac{1}{3} R_{mm} \delta_{ij} + {}_D R_{ij}$$

where δ_{ij} is again the Kronecker delta. The isotropic part, $R_{mm} \equiv \widetilde{u''_m u''_m}$, of the Reynolds subgrid scale stress tensor can be absorbed into the pressure. In many flows, it is an order of magnitude smaller than the thermodynamic pressure so it has been neglected in many applications. During the last decade, Yohizawa (1986) developed a model for R_{mm} which is given by

$$R_{mm} = -2 C_I \overline{\rho} \Delta^2 \tilde{S}_{mn} \tilde{S}_{mn} \tag{22}$$

where C_I is a constant. Speziale, Erlebacher, Zang and Hussaini (1988) showed that this proposed model performs poorly. A scatterplot of this model compared with DNS is shown in Figure 1 showing the poor level of correlation.

The Smagorinsky model has several deficiencies that can be summarized as follows:

(1) The Smagorinsky constant is not in reality a constant. It can vary by as much as a factor of two or three from flow to flow. This is because the Smagorinsky model is badly parameterized (see Speziale 1997a). Furthermore, it only correlates with DNS

at the 50% level. To get an idea of how poor this result is, the correlation between the functions $y = x$ and $y = e^{-x}$ on the interval [0, 1] is more than 50% despite the fact that they are qualitatively different functions (one is monotonically increasing while the other is monotonically decreasing)!

(2) The Smagorinsky model *does not* depend on rotational strains through the invariant $\xi \propto (\tilde{W}_{ij}\tilde{W}_{ij})^{1/2}$ ($\tilde{W}_{ij} \equiv \frac{1}{2}(\partial\tilde{u}_i/\partial x_j - \partial\tilde{u}_j/\partial x_i)$ is the Favre-filtered vorticity tensor) and, furthermore, has the wrong dependence on the irrotational strain rate invariant $\eta \propto (\tilde{S}_{ij}\overline{S}_{ij})^{1/2}$. For Reynolds stress models in equilibrium, the eddy viscosity reduces to

$$\nu_T \propto \frac{3}{3 - 2\eta^2 + 6\xi^2}$$

(see Gatski and Speziale 1993).

(3) The dependence on the computational mesh size Δ should be through the dimensionless ratio Δ/L_K. *What determines how well a computation is resolved in the numerical simulation of turbulence is whether or not the grid size is small (or large) compared to the Kolmogorov length scale.* The dimensional dependence on Δ in the Smagorinsky model is simply incorrect. In the Smagorinsky model, $\tau_{ij} \to \infty$ as $\Delta \to \infty$. Hence, a badly calibrated Reynolds stress model is obtained in the coarse mesh limit. The model becomes far too dissipative as the mesh becomes coarse.

In so far as point (2) is concerned, this makes it impossible for the Smagorinsky model to properly describe rotating flows. For example, it is well known that in an incompressible rapidly rotating isotropic turbulence, the cascade is essentially shut off so that the turbulence undergoes a linearly viscous decay (see Speziale, Mansour and Rogallo 1987). Hence, it is possible to conduct direct simulations even at high turbulence Reynolds numbers. The Smagorinsky model is far too dissipative in this case where it can yield results that are completely erroneous. For a rapidly rotating isotropic turbulence, the Smagorinsky constant is essentially zero except, perhaps, at astronomically high Reynolds numbers or for extremely coarse meshes.

In the next section, a new methodology for the large-eddy simulation of compressible turbulent flows will be presented. There is no question that a new approach that transcends the Smagorinsky model is needed. Even the dynamic subgrid scale model of Germano, Piomelli, Moin and Cabot (1991) does not overcome these shortcomings as discussed in Speziale (1997a).

3. A NEW APPROACH TO COMPRESSIBLE LARGE-EDDY SIMULATIONS

The new approach to compressible LES that is being proposed has subgrid scale stress models that are of the following form:

$$\tau_{ij} = [1 - exp(-\beta\Delta/L_K)]^n \left[\frac{2}{3}K\delta_{ij} - \alpha_1 f(\eta,\xi)\frac{K^2}{\mathcal{E}}(\tilde{S}_{ij} - \frac{1}{3}\tilde{S}_{mm}\delta_{ij})\right] + \tau_{ij}^A \tag{23}$$

where τ_{ij}^A represents the anisotropic part of the subgrid scale stress tensor. Here, an overtilde represents a Favre-filter whereas

$$\eta = \alpha_2(\tilde{S}_{ij}\tilde{S}_{ij})^{1/2}\frac{K}{\mathcal{E}}, \quad \xi = \alpha_3(\tilde{W}_{ij}\tilde{W}_{ij})^{1/2}\frac{K}{\mathcal{E}} \tag{24}$$

where $\tilde{S}_{ij}$ and $\tilde{W}_{ij}$ are the Favre-filtered rate of strain and vorticity tensors, Δ is the computational mesh size, $L_K \equiv \overline{\nu}^{3/4}/\mathcal{E}^{1/4}$ (where $\overline{\nu} \equiv \overline{\mu}/\overline{\rho}$) is the Kolmogorov length scale, and β, n, α_1, α_2 and α_3 are constants (α_1, α_2 and α_3 are obtained from a Reynolds stress model along with the function f). Here, K and $\mathcal{E}$ represent the *Reynolds-averaged* turbulent kinetic energy and dissipation rate obtained from a *Reynolds stress calculation* with the two-equation model equivalent to that given above in the coarse mesh limit as $\Delta/L_K \to \infty$.

In the coarse mesh limit, a Reynolds stress model given by

$$\tau_{ij}^{(R)} = \frac{2}{3}K\delta_{ij} - \alpha_1 f(\eta,\xi)\frac{K^2}{\mathcal{E}}(\tilde{S}_{ij} - \frac{1}{3}\tilde{S}_{mm}\delta_{ij}) + \tau_{ij}^{(R)A} \tag{25}$$

is recovered which is an explicit algebraic stress model (see Gatski and Speziale 1993 and Speziale 1996 for the compressible extension of this model). The turbulent dissipation rate $\mathcal{E}$ – and, hence, the turbulent kinetic energy K – have to be obtained anyway in order to get an estimate of the Kolmogorov length scale L_K. Since, the Kolmogorov length scale $L_K = \overline{\nu}^{3/4}/\mathcal{E}^{1/4}$, the dissipation rate only has to be estimated to within 50% with the modeled dissipation rate equation to get a good estimate of the Kolmogorov length scale (the dissipation rate is raised to the 1/4 power as mentioned before). This is quite feasible with state-of-the-art Reynolds stress models. Thus, this methodology requires that a RANS calculation be done in parallel with the LES. This will, in most circumstances, only add at most 10% to the computational expense. Here, we parameterize the model in terms of the Reynolds-averaged turbulent kinetic energy and dissipation rate since the subgrid scale turbulent kinetic energy and dissipation rate can vary too much locally. This model has been written before in the shorthand notation as (see Speziale 1997b)

$$\tau_{ij} = [1 - exp(-\beta\Delta/L_K)]^n \tau_{ij}^{(R)} \tag{26}$$

where $\tau_{ij}^{(R)}$ is a Reynolds stress model that is written partially in terms of filtered fields. An explicit algebraic stress model is used for this purpose as discussed above.

The anisotropic eddy viscosity terms take the form

$$\tau_{ij}^A = [1 - exp(-\beta\Delta/L_K)]^n [\alpha_4 \frac{K^3}{\mathcal{E}^2} f(\eta,\xi)(\tilde{W}_{ik}\tilde{S}_{kj} + \tilde{W}_{jk}\tilde{S}_{ki})$$

$$+\alpha_5 f(\eta,\xi)\frac{K^3}{\mathcal{E}^2}(\tilde{S}_{ik}\tilde{S}_{kj} - \frac{1}{3}\tilde{S}_{kl}\tilde{S}_{kl}\delta_{ij})] \tag{27}$$

where again the overtilde represents a Favre-filtered quantity whereas K and $\mathcal{E}$ are the Reynolds-averaged turbulent kinetic energy and dissipation rate obtained from a Reynolds stress calculation (α_4 and α_5 are constants). In the coarse mesh limit as $\Delta/L_K \to \infty$, the anisotropic eddy viscosity terms of an explicit algebraic stress model are recovered, extended to compressible flows (see Gatski and Speziale 1993 and Speziale 1996). These terms are dispersive in character and can account for backscatter effects (cf., Clark, Ferziger and Reynolds 1979)

For incompressible Reynolds stress models in equilibrium

$$f(\eta,\xi) = \frac{3}{3 - 2\eta^2 + 6\xi^2}. \tag{28}$$

A singularity can occur when this expression is applied to turbulent flows where there are significant departures from equilibrium. Gatski and Speziale (1993) introduced the simple regularization

$$\frac{3}{3 - 2\eta^2 + 6\xi^2} \approx \frac{3(1+\eta^2)}{3 + \eta^2 + 6\xi^2\eta^2 + 6\xi^2} \tag{29}$$

which is obtained by a Taylor series expansion. For turbulent flows in equilibrium where $\eta, \xi < 1$, it yields results that are indistinguishable from (28) where it formally applies. But it is regular and computable for *all* values of η and ξ. More recently, Speziale and Xu (1996) obtained expressions via a formal Pade$'$ approximation that builds in some limited agreement with the Rapid Distortion Theory (RDT) solutions for plane shear and plane strain turbulence. The constants in this Reynolds stress model are given by

$$\alpha_1 = 0.374, \quad \alpha_2 = 0.145, \quad \alpha_3 = 0.308, \tag{30}$$

$$\alpha_4 = 0.115, \quad \alpha_5 = 0.108. \tag{31}$$

These constants are based on benchmark flows in the incompressible limit since the Morkovin hypothesis is being applied where compressible models are a variable density extension of their incompressible counterparts.

The Reynolds-averaged turbulent kinetic energy K and dissipation rate $\mathcal{E}$ are obtained from modeled versions of their transport equations which take the compressible form (cf. Speziale 1996 and Speziale and Sarkar 1991):

$$\begin{aligned} \frac{\partial}{\partial t}(\overline{\rho}K) + (\overline{\rho}\tilde{u}_i K)_{,i} = &-\overline{\rho}\tau_{ij}^{(R)}\tilde{u}_{i,j} - \overline{\rho}(\mathcal{E} + \overline{p' u'_{i,i}} \\ &-\overline{u''_i}\overline{p}_{,i} + \overline{u''_i}\overline{\sigma}_{ij,j} + \left[\left(\overline{\mu} + \frac{\overline{\mu}_T}{\sigma_K}\right) K_{,i}\right]_{,i} \end{aligned} \tag{32}$$

$$\begin{aligned} \frac{\partial}{\partial t}(\overline{\rho}\mathcal{E}) + (\overline{\rho}\tilde{u}_i\mathcal{E})_{,i} = &-C_{\varepsilon 1}\overline{\rho}\frac{\mathcal{E}}{K}\tau_{ij}^{(R)}\left(\tilde{u}_{i,j} - \frac{1}{3}\tilde{u}_{k,k}\delta_{ij}\right) \\ &-\frac{4}{3}\overline{\rho}\mathcal{E}\tilde{u}_{i,i} - C_{\varepsilon 2}\overline{\rho}\frac{\mathcal{E}^2}{K} + \left[\left(\overline{\mu} + \frac{\overline{\mu}_T}{\sigma_{\mathcal{E}}}\right)\mathcal{E}_{,i}\right]_{,i} \end{aligned} \tag{33}$$

where $\mathcal{P} \equiv -\tau_{ij}^{(R)}\partial\tilde{u}_i/\partial x_j$ is the turbulence production, $\overline{\mu}_T = C_\mu\overline{\rho}K^2/\mathcal{E}$ is the eddy viscosity and C_μ, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$, σ_K and $\sigma_{\mathcal{E}}$ are constants that assume the values of 0.09, 1.44, 1.83, 1.0 and 1.3, respectively. These equations have served as a cornerstone for two-equation models in the incompressible limit. In order to integrate this model to a wall it is only necessary to remove the singularity in the destruction term that appears on the right-hand-side of (33) with the coefficient $C_{\varepsilon 2}$ (see Speziale and Abid 1995). *No ad hoc wall damping functions are needed in the Reynolds stress model.* This is accomplished by replacing $C_{\varepsilon 2}$ with the term

$$C_{\varepsilon 2}[1 - exp(-R_y/10)] \tag{34}$$

where $R_y = K^{1/2}y/\overline{\nu}$ given that y is the coordinate normal to the wall. In many applications, a small vortex stretching term has been added to (33) to make the calculations better behaved. It removes the singularity in plane stagnation point turbulent flows and, furthermore, allows for the description of both the log-layer and homogeneous turbulence in equilibrium with a simple unified model where it is not necessary to solve the cubic equation arising out of the consisistency condition (see Abid and Speziale 1996 and Speziale, Jongen and Gatski 1997). The dilatational dissipation has been neglected since it leads to a degradation of the results in wall-bounded flows (see Speziale 1996). The dilatational dissipation was proposed by Zeman (1990) and Sarkar, Erlebacher, Hussaini and Kreiss (1991) largely based on free turbulent shear flows.

It is worthwhile to note that these equations are consistent with the limit of compressed isotropic turbulence. For this problem, the mean velocity gradient tensor is given by

$$\bar{u}_{i,j} = \begin{pmatrix} \frac{1}{3}\Gamma & 0 & 0 \\ 0 & \frac{1}{3}\Gamma & 0 \\ 0 & 0 & \frac{1}{3}\Gamma \end{pmatrix} \tag{35}$$

where Γ is the expansion/compression rate which is constant. The model provided herein reduces approximately to the simple coupled ODE's:

$$\dot{K} = -\frac{2}{3}\Gamma K \tag{36}$$

$$\dot{\mathcal{E}} = -\frac{4}{3}\Gamma \mathcal{E} \tag{37}$$

for $|\Gamma| K_0/\mathcal{E}_0 \gg 1$. The short-time solution to Eqs. (36) - (37) is given by:

$$K = K_0 \exp\left(-\frac{2}{3}\Gamma t\right) \tag{38}$$

$$\mathcal{E} = \mathcal{E}_0 \exp\left(-\frac{4}{3}\Gamma t\right) \tag{39}$$

$$\Lambda = \Lambda_0 \exp\left(\frac{1}{3}\Gamma t\right) \tag{40}$$

where $\Lambda \equiv K^{3/2}/\mathcal{E}$ is the integral length scale. *These are identical to the results obtained by Reynolds (1987) based on Rapid Distortion Theory (RDT).* In contrast to these results, a variable density extension of the commonly used second-order closures erroneously predicts that

$$\Lambda = \Lambda_0 \exp(-0.04\Gamma t) \tag{41}$$

(see Reynolds 1987). According to (41), the integral length scale will *decrease* under an expansion ($\Gamma > 0$) and *increase* under a compression ($\Gamma < 0$) – results that are clearly in error as first pointed out by Reynolds (1987).

It is also worth noting that in a rapidly rotating incompressible isotropic turbulence, $f(\eta, \xi) \to 0$ so $\tau_{ij} \to 0$ yielding a DNS. This results from the fact that

$$\tilde{W}_{ij} = \frac{1}{2}\left(\frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial \tilde{u}_j}{\partial x_i}\right) + e_{mji}\Omega_m \tag{42}$$

in rotating frames where Ω_m is the rotation rate of the frame and e_{mji} is the permutation tensor (hence, $\xi \sim \Omega$ in a rapidly rotating flow with angular velocity Ω). As mentioned earlier, in a rapidly rotating incompressible isotropic turbulence the energy cascade is essentially shut off so that direct numerical simulations can be conducted with a 128^3 mesh even at high turbulence Reynolds numbers. A 128^3 mesh forms a cornerstone of this new approach to LES as will soon be discussed. In contrast, the Smagorinsky model is far too dissipative so it yields incorrect results for this problem.

The grid function

$$[1 - exp(-\beta\Delta/L_K)]^n \tag{43}$$

bridges the gap between DNS, LES and RANS where L_K is the Kolmogorov length scale $L_K = \bar{\nu}^{3/4}/\mathcal{E}^{1/4}$ estimated from a Reynolds stress calculation (again, Δ is the computational mesh size). In the limit as $\Delta/L_K \to \infty$ the grid function goes to one and we recover a Reynolds stress model whereas in the limit as $\Delta/L_K \to 0$, it goes to zero and we formally recover a DNS. Actually, when Δ/L_K is of order one, we should have a DNS (this has been built into the calibration). Since $L_K \equiv R_t{}^{-3/4}K^{3/2}/\mathcal{E}$ where $R_t \equiv K^2/\bar{\nu}\mathcal{E}$ is the turbulence Reynolds number, $\Delta/L_K \to \infty$ as $R_t \to \infty$ (thus, we recover a Reynolds stress model in the coarse mesh/infinite-Reynolds-number limit). For the initial calculations, n has been taken to be one and β has been calibrated as follows:

$$\beta \approx 0.001. \tag{44}$$

A power law for the grid function has been theoretically obtained using Renormalization Group methods (Woodruff and Hussaini, *Private Communication*). Note that for $\Delta/L_K <$ 100, we approximately obtain a power law from (43) via a Taylor expansion. Most practical LES are conducted for $\Delta/L_K = 10 - 100$.

The modeling of the other higher-order correlations that are needed for the closure of the compressible equations is along the same lines as that for the Reynolds stress models. In effect, for this approach, a subgrid scale model is nothing more than a scaled down version of the Reynolds stress model – scaled down by the grid function to have less dissipation. For the subgrid scale heat flux

$$\widetilde{u_i''T''} = -[1 - exp(-\beta\Delta/L_K)]^n \frac{C_\mu}{Pr_T}\frac{K^2}{\varepsilon}\tilde{T}_{,i} \tag{45}$$

The turbulent Prandtl number $Pr_T \approx 0.9$. In the coarse mesh limit, as the grid function goes to one, the standard gradient transport model for the Reynolds heat flux is recovered. The same is true of the subgid scale mass flux which is modeled as

$$\overline{u_i''} = [1 - exp(-\beta\Delta/L_K)]^n \frac{C_\mu}{\overline{\rho}\sigma_\rho} \frac{K^2}{\varepsilon} \overline{\rho}_{,i} \tag{46}$$

(see Cebeci and Smith 1974). Here, the constant σ_ρ is approximately equal to 0.5. The subgrid scale dissipation ε and Reynolds-averaged dissipation $\mathcal{E}$ are related by the grid function as follows

$$\varepsilon = [1 - exp(-\beta\Delta/L_K)]^n \mathcal{E}. \tag{47}$$

The pressure-dilatation correlation is modeled as

$$\overline{p' u'_{i,i}} = [1 - exp(-\beta\Delta/L_K)]^n \{a_2 \overline{\rho} \tau_{ij} \tilde{u}_{i,j} M_t + a_3 \overline{\rho} \varepsilon M_t^2\} \tag{48}$$

where

$$a_2 = 0.15, \quad a_3 = 0.2 \tag{49}$$

and

$$M_t \equiv (2K/\gamma R\tilde{T})^{1/2} \tag{50}$$

is the turbulence Mach number (γ is the ratio of specific heats and R is the ideal gas constant). In the coarse mesh limit, as the grid function goes to one, a recently proposed Reynolds-averaged model is obtained for the pressure-dilatation correlation that is suitable for compressible shear flows (see Sarkar 1992). Thus, we have a complete closure to the compressible filtered equations of motion. The full Reynolds stress model that is recovered in the coarse mesh limit has been tested successfully in a variety of benchmark compressible flows (see Speziale 1996).

Some comments are needed concerning the choice of a filter in this new approach to large-eddy simulations and the melding together of spatial filtering in LES and Reynolds averaging in RANS. We want a filter that yields the minimum contamination of the large scales. The reason for this is clear; defiltering must be avoided since it constitutes an ill-posed mathematical problem (see Speziale 1997b). The purpose of practical LES is to predict the Reynolds-averaged fields. In order to do so, the filtered velocity, which is calculated, must invariably be used to estimate the large-scale part of the instantaneous velocity which then yields the Reynolds-averaged fields through appropriate ensemble or time averages. The filtered equations of motion (11)–(13) are of the same form as the Reynolds-averaged equations. In the coarse mesh limit, the ramp function will be one and the model will be so dissipative that a RANS calculation will be automatically recovered with a state-of-the-art Reynolds stress model. It is envisioned that ensemble averages will be taken even if we are conducting a time-dependent RANS. Thus, we do not need to know the effect of the filter – which can never be fully known in complex geometries – except, perhaps for model calibration in benchmark flows. This allows us to meld together the LES and RANS methodologies which are normally treated as disparate approaches. In both of these approaches we calculate what is tantamount to the large-scale velocity field – through the same basic equations of motion – and then obtain the Reynolds-averaged fields through ensemble averages (time averages in a statistically steady turbulence). The large scales make the dominant contribution to the most pertinent fields such as the turbulent kinetic energy. A minimum contamination of the large scales can be accomplished with, of the order of, a 128^3 computational mesh using a filter with a compact support – such as the box filter – which has a small filter width of, for example, two mesh points. Some of the previously conducted coarse grid LES (which has typically had no more than 32^3 mesh points) must be avoided wherein the filter width has, at times, been as much as 25% of the computational domain, significantly contaminating the large scales. Besides, recent increases in computational capacity have begun to make 128^3 computations much more feasible for engineering calculations (a small compromise to 100^3 computations can always be made). In addition, it should be noted that practical LES – in complex geometries – will require the use of finite difference techniques with a compact filter where we will never make explicit use of the filter. These finite difference methods should, furthermore, be based on fourth-order accurate finite difference schemes for better accuracy. Spectral methods have to be abandoned if complex turbulent flows are to be addressed. With this new methodology, the gap between DNS, LES and RANS can be bridged (see Figure 2).

4. CONCLUSION

A new approach to the large-eddy simulation of the high-speed compressible turbulent flows of technological importance has been proposed. In this new methodology, subgrid scale models go continuously to Reynolds stress models in the coarse mesh/infinite Reynolds number limit. Hence, with this new methodology it is possible to achieve the long held dream of going continuously from a large-eddy simulation to a Reynolds stress calculation as the mesh becomes coarse or the Reynolds number becomes extremely large. It is firmly believed that in complex wall-bounded turbulent flows – especially with flow separation where wall functions cannot be used – the best that one can do, at this time, for the extremely high Reynolds numbers encountered in many technological applications (such as some naval flows where $Re \sim O(10^9)$) is a RANS computation since the crucial wall layer cannot be resolved. At more moderate Reynolds numbers, LES is possible (of course, at low turbulence Reynolds numbers it is possible to conduct a DNS). The RANS model that was presented in this study is a two-equation model that contains some of the most recent developments in compressible turbulence modeling. In the incompressible limit it collapses to an explicit algebraic stress model which is a two-equation model that is consistent with a state-of-the-art second-order closure model in the limit of homogeneous turbulence in equilibrium. A new approach is unquestionably needed that transcends the Smagorinsky model. The Smagorinsky model has a variety of deficiencies as outlined in this paper (also see Speziale 1997a). The only reason to believe that it has been successful in previous applications is because it drains enough energy to approximately account for the energy cascade to the scales that are left unresolved – an effect that is achieved by the *ad hoc* adjustment of the Smagorinsky constant.

Some brief remarks are in order concerning the role of direct and large-eddy simulations in turbulence. There is no question that DNS – and the computer in general – has revolutionized the study of turbulence. DNS has already shed new light on the physics of a range of basic turbulent flows and the future potential is enormous. It already appears that in the not too distant future, DNS will entirely replace basic benchmark physical experiments for homogeneous turbulence, near-wall turbulent flows and basic compressible flows at lower turbulence Reynolds numbers. However, it appears that DNS will, for a long time to come, be limited to relatively simple geometries and low to moderate turbulence Reynolds numbers. Direct simulations of the complex turbulent flows of technological importance, at high turbulence Reynolds numbers, could require the generation of data bases with upwards of 10^{20} numbers. Thus, it is crucial that large-eddy simulations be made to work. As far as LES is concerned, it must be said that it has never lived up to its initial promise. The way that traditional LES has been formulated is not predictive and is probably only suitable for doing less expensive parametric studies of benchmark direct simulations once the reliability of the subgrid scale model has been established by DNS for the baseline case. In order to solve the complex turbulent flows of technological importance, an entirely new approach to LES is direly needed.

Finally, some comments are warranted concerning supersonic turbulent flows – particularly in wall-bounded geometries. Since there is considerable heating in these flows, the effective Reynolds number (through a rise in the kinematic viscosity) is not extremely large even in many of the high-speed compressible flows of technological importance. Thus, the prospects for being able to conduct a large-eddy simulation in many practical flow situations are fairly good for compressible turbulence. This would include the flow around high-speed aircraft and missiles to name just a few applications. For those cases where LES is not feasible, a time-dependent RANS can be always be conducted which is expected to be far superior to traditional steady RANS. The methodology discussed in this paper has the potential to make a significant impact on these problems and to bridge the gap between DNS, LES and RANS.

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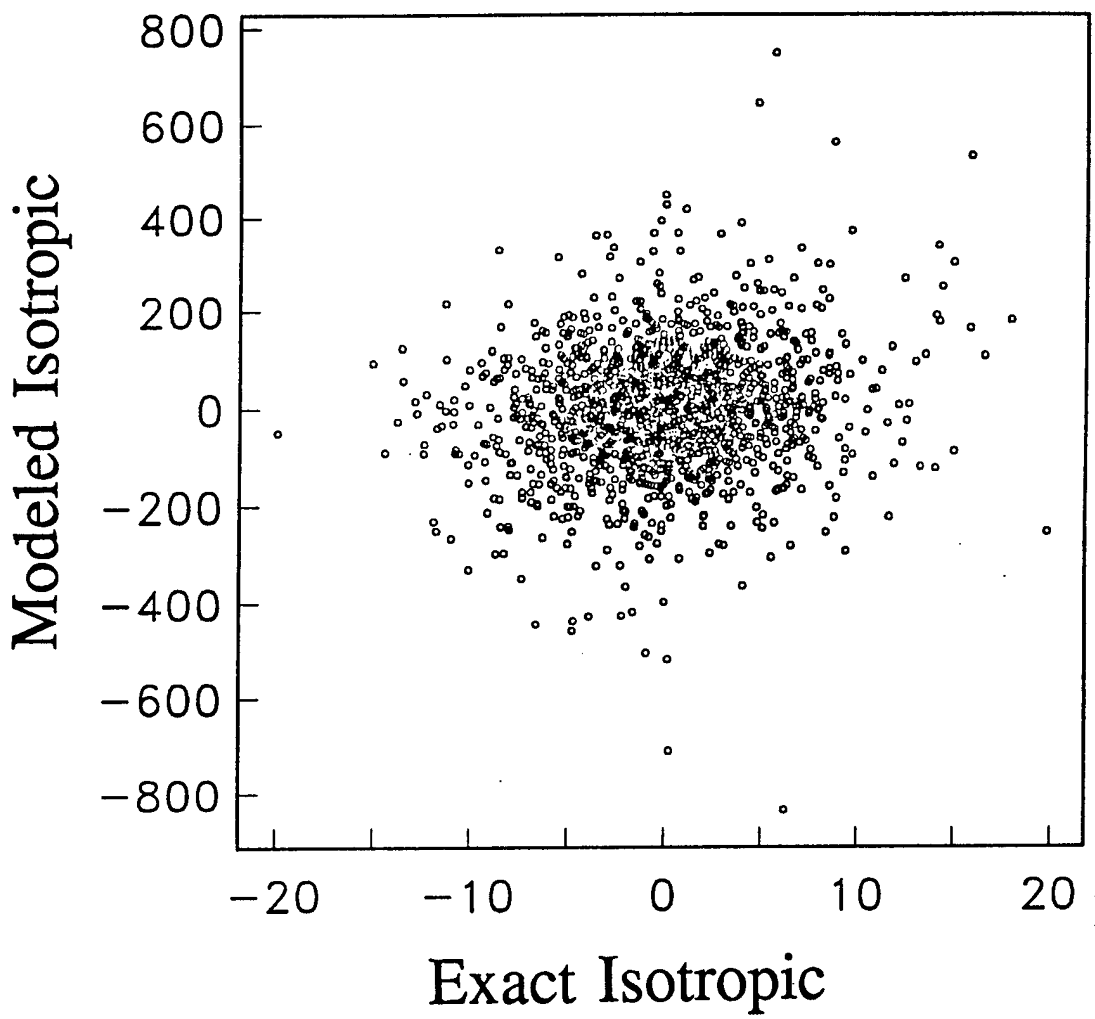

Figure 1. Scatterplot of the Yoshizawa (1986) model for R_{mm} versus the exact subgrid scale isotropic stress obtained from a 96^3 direct numerical simulation of compressible isotropic turbulence at a Mach number of 0.1. (Taken from Speziale *et al* 1988).

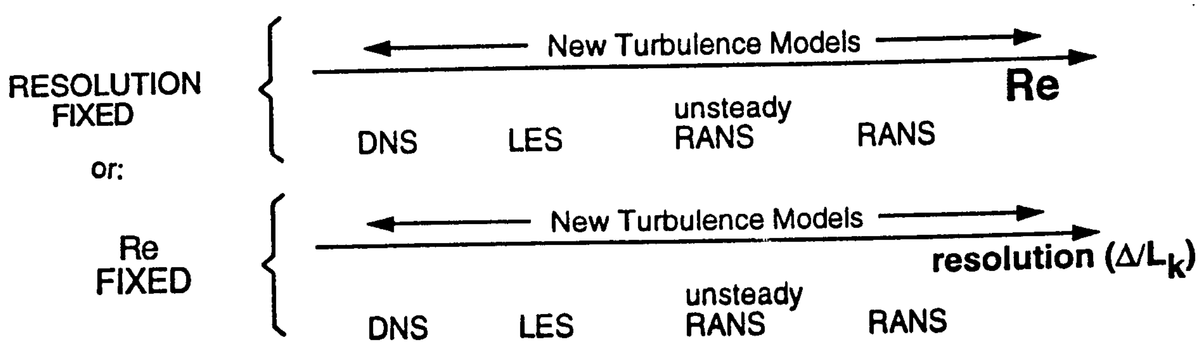

Figure 2. Schematic diagram of numerical simulations in turbulence. (Provided by H. Fasel, University of Arizona).

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13. ABSTRACT *(Maximum 200 words)*

An entirely new approach to the large-eddy simulation (LES) of high-speed compressible turbulent flows is presented. In this new approach to large-eddy simulations, subgrid scale stress models go continuously to Reynolds stress models in the coarse mesh/infinite Reynolds number limit, where a Reynolds stress calculation (RANS) is done in parallel with the LES to get an estimate of the Kolmogorov length scale. Hence, this formally constitutes a combined LES/time-dependent RANS capability. Here, the Reynolds stress model that is recovered in the coarse mesh limit has a dependence on rotational strains through strain-dependent coefficients as well as through anisotropic eddy viscosity terms which are usually neglected in subgrid scale models. Unlike in existing subgrid scale models, this new model has the correct dependence on the mesh size through the dimensionless ratio of the computational mesh size to the Kolmogorov length scale. It is this ratio that determines how well-resolved a computation is in the numerical simulation of turbulence and should be used to parameterize subgid scale models. Use is made of the Morkovin hypothesis in the formulation of compressible subgrid scale models. This allows for the description of supersonic turbulent flows provided that they are not in the hypersonic flow regime. A critical assessment of this new approach is provided along with a discussion of traditional approaches and the prospects for future applications to the high-speed compressible flows of technological importance.

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